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Spatial structure of phosphorus-containing heterocycles - Communication 28. Conformation of phenyl radical in 5-phenyl-5-oxo-1,3,5-dioxaphosphorinanes and thiono analogs

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Abstract

1. On the basis of data on the Kerr effect in solutions, the stereoisomers of 5-phenyl-5-oxo- and 5-phenyl-5-thiono-2,4,6-trimethyl-1,3,5-dioxaphosphorinanes, differing in the position of the exocyclic substituents on the P atom, are characterized by nearly parallel orientation of the plane of the benzene ring and the plane of the bonds {Mathematical expression}. In the conformation that we have found, optimal structural conditions are realized for resonance interaction of the π-orbitals of the phenyl radical and the P=X bond. 2. This sort of interaction in the UV spectra is manifested in a bathochromic shift of the benzene absorption bands (particularly λ2) and their intensification. In the sulfides, the absorption bands of the benzene overlap those of the thiophosphoryl group. © 1982 Plenum Publishing Corporation.

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